JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS

ELSEVIER Journal of Computational and Applied Mathematics 75 (1996) 171–195

On the error and its control in a two-parameter generalised Newton–Cotes rule

Ulf Torsten Ehrenmark *

Department CISM, London Guildhall University, 100 Minories, London EC3 N1JY, United Kingdom

Received 14 July 1995; revised 21 May 1996

Abstract

A quadrature formula containing two free (phase) parameters k, k', and recently written by Van Daele et al. [13], is rederived using an extension of Lagrange's identity. By using this method, a closed-form expression is determined for the local error term $E[f]$ and the relevant Peano kernel is given explicitly. Sufficient conditions are established, under which this kernel remains *definite*, thus allowing a particularly simple expression to be deduced for $E[f]$ which reduces to the classical result for Boole's rule in the limit $k, k' \to 0$.

Recent work on optimisation of global error is extended to include the new rule. It is shown that this error can be reduced by a factor $O(h^2)$ on a certain curve in the phase space. A further reduction by a factor $O(h^2)$ is sometimes possible by choosing the phase parameters on the intersection of this curve and another such. When these curves intersect only at complex values, the reduction is still achieved. A closed-form expression for the global error is also derived under these circumstances and this is seen to be asymptotically $O(h^{10})$ as $h \to 0$.

A second limiting form of the five-point formula is found to reduce to the generalised Boole's rule written by Vanden Berghe et al. [14] and a third limiting form is also written. This third rule, which is a special case of a one-parameter family of generalised Boole's rules, is seen to perform better than the other two in the two examples studied.

Several numerical examples are given, with extensive diagrams, to illustrate all uses of the techniques proposed.

Keywords: Lagrange's identity; Peano kernel; Boole's rule; Newton–Cotes quadrature; mixed interpolation

AMS classification: 65D30

1. Introduction

Generalisations of Newton–Cotes quadrature rules, which introduce an element of trigonometric interpolation, have begun to appear (e.g. [4] or [14]) following the successful use of such interpolation in constructing linear operators numerically to integrate a class of Schrödinger equations, e.g. [11]. The three-point formula given by Ehrenmark [4], which is based on a single free parameter k, has been successfully employed in a number of hydrodynamic situations, e.g. [6]. Meanwhile, De Meyer

* E-mail: ute@titus.lgu.ac.uk.

PII S0377-0427(96)00085-4

et al. [3] had placed the mixed interpolation in a rigorous framework and more recent applications of the ideas introduced include the exploitation of trigonometric "hat" functions in approximation theory [15]. Also, very recently, Bocher et al. [1] have applied the three-point formula to construct an improved solver for Volterra equations of the second kind. The above authors used a variety of methods, some discussed below, for choosing the free parameter in an optimum way to minimise local truncation error. It was Köhler [10], who first noticed that it was indeed possible to optimise the global error by a single choice of this free parameter. Aspects of this are discussed in some detail later.

A quadrature formula with *two* free parameters, based on mixed interpolation on five equally spaced points, was first published by Van Daele et al. [13] as a special case of a more general construction on $n+1$ points. In the latter case, an interpolant $f_n(x)$ was determined for $f(x) \in C^{n+1}(I)$, where I is the intended integration interval, which was a linear combination of $\cos kx$, $\sin kx$, $\cos k'x$, $\sin k'x$ and a polynomial of degree $n-4$. For the case $n=4$ this interpolant was then integrated over the "panel" $(0, 4h)$ to yield the quadrature approximant. However, the integration was not undertaken also of $f_n - f$ to yield a local truncation error for the rule, the authors being content to note that this error would be proportional to an expression involving the first three even-ordered derivatives $(f'', f^{(\mathrm{iv})}$ and $f^{(\mathrm{vi})})$ at some point $x = \eta$ in the panel. Details of this are given below.

One objective of the present work is to obtain a closed-form expression for the local total truncation error (ltte) and a new derivation of the formula, using an extension of Lagrange's identity given in [2, p.239], yields a suitable framework for doing this. At the same time the formula itself emerges in a form which (unlike the form given in [13]) is not expressed as a "correction" to the equivalent Newton–Cotes rule (Boole's rule) but is instead written in a composite form which makes it more amenable to fast coding. The formula for the ltte is seen to reduce to the error of the standard Newton–Cotes five-point (Boole's) rule in the limit of both free parameters tending to zero.

A second objective here being the optimisation of parameter choice through global error examination, it is thought prudent to begin with a derivation of the three-point rule, first derived in [4], but here using the extension to Lagrange's identity. This rule was discussed also by Köhler [10], who pioneered the technique for chosing an optimum parameter, with respect to global error, in certain situations. However, the linear operator which generates the five-point rule presently being investigated, does not strictly belong to the class considered by Köhler. The revised study will give us the opportunity of generalising the optimisation strategy and it will be seen that Köhler's technique can be extended to the new formula. In doing this, the relevant Peano kernel is written explicitly and a closed-form expression is obtained finally for the global error in a given application.

A feature of the global error optimisation procedure is that we obtain successive error reductions each of $O(h^2)$, where h is the local step length, on two curves in the parameter space, provided these curves intersect. Examples are given to show that sometimes they do intersect and sometimes they do not. Nevertheless, in the latter case they may intersect in complex values of the parameters. Previous authors e.g. Van Daele et al. [13] have shown that the quadrature rule may be applied with complex (conjugate) values of the parameters. The complication of redefining the coefficients of the quadrature rule in terms of hyperbolic functions, undertaken by those authors, does not however seem necessary here when using a global strategy. Provided the coding is changed to allow for complex variables, the computation seems to proceed perfectly normally using a universal definition of the coefficients. This may be contrasted with the local strategies used in e.g. [13] or [14]. This is illustrated with some examples herein.

The layout of the paper is as follows. The extension of Lagrange's identity is written in Section 2 and the application to the three-point rule is discussed in full with the local error term (closed-form expression) recovered. The five-point rule and its error is similarly derived in Section 3. In Section 4 is examined the application of an optimisation strategy to reduce the global error in applications. The result is stated there in the form of a theorem which indicates that, subject to a number of restrictions, careful choice of the two free parameters can reduce global error by a factor of $O(h^4)$, leaving an expression which is $O(h^{10})$ *asymptotically as* $h \to 0$. In Section 5, we present various numerical examples to illustrate the ideas described and some of the results are compared with those of earlier authors e.g. Van Daele et al. [13]. Some concluding remarks, including a new single-parameter Boole's rule derived from the limit $k' \to k$, are given in Section 6. This new rule is tested for two examples and these indicate that (i) the new rule gives improved results over the old rule for the more oscillatory functions and (ii) the application of Köhler's [10] global parameter optimisation strategy is seen to be superior to the method of local choice of parameter used in e.g. [14] or [13].

2. The three-point rule

We begin by writing the extension of Lagrange's identity as given in [2, p.293] for a function $f \in AC^{n-1}[a,b]$ and a weight $w \in L_1[a,b]$:

$$\int_a^b w(x)f(x)\,dx = -\sum_{i=0}^{m}\left[\sum_{k=0}^{n-1} f^{(k)}(x)L_{n-k-1}^{*}\{\phi_i(x)\}\right]_{x_i}^{x_{i+1}} + \sum_{i=0}^{m}\int_{x_i}^{x_{i+1}} \phi_i(x)L\{f\}\,dx. \tag{2.1}$$

In this formula, L_r is the rth-order differential operator

$$L_r = D^r + a_1(x)D^{r-1} + \cdots + a_{r-1}(x)D + a_r(x), \quad r = 0,1,\ldots,n-1,$$

L_r^* is its adjoint and L coincides with L_r on setting $r=n$. Also $w(x)$ is a suitable weight function and the functions $\{\phi_i(x)\}$ are any solutions of $L^*(\phi) = w(x)$. It is further assumed that the coefficients $a_k(x) \in AC^{n-k-1}[a,b]$, $k = 1,2,\ldots,n-1$, $a_n(x) \in L_1[a,b]$ and the partition used is such that $a = x_0 < x_1 < \cdots < x_{m-1} < x_m = b$.

In considering the application first to the three-point one-parameter (λ) rule, earlier written in [7] in unpublished work and formalised in [4], it is necessary to point out that such a rule appears to have been first given by Ghizetti and Ossicini [8, p.89] but only for the special case $\lambda=1$. Moreover, error bounds were only given for the remainder term in a single panel application.

We set $m = 1$, $w(x) \equiv 1$, $n = 3$ and note that the fundamental operator required is

$$L_n \equiv L \equiv D^3 + \lambda^2 D.$$

This operator is null on the set $S_3(\lambda)$ spanned by $\{1, \sin\lambda x, \cos\lambda x\}$ so the remainder term of (2.1) vanishes for all $f \in S_3(\lambda)$. The subordinate operators are $L_2 = D^2 + \lambda^2$, $L_1 = D$ and $L_0 = 1$. The solutions to $L^*(\phi) = w(x)$ are taken in the form

$$\phi_0 = A\sin\lambda x + B\cos\lambda x + C - x/\lambda^2,$$

$$\phi_1 = \bar{A}\sin\lambda x + \bar{B}\cos\lambda x + \bar{C} - x/\lambda^2,$$

and the constants are chosen to satisfy

$$L_{n-k-1}\phi_0(x_0) = 0, \quad k = 1,\dots,n-1,$$

$$L_{n-k-1}\phi_1(x_2) = 0, \quad k = 1,\dots,n-1,$$

$$L_{n-k-1}\phi_0(x_1) = L_{n-k-1}\phi_1(x_1), \quad k = 1,\dots,n-1,$$

where $x_j = (j-1)h$. With these three equations satisfied, Eq. (2.1) reduces to the "local" quadrature rule

$$\int_{-h}^{h} f(x)\,\mathrm{d}x = -[f(x)L_2^*\{\phi_0(x)\}]_{x_0}^{x_1} - [f(x)L_2^*\{\phi_1(x)\}]_{x_1}^{x_2} + R, \tag{2.2}$$

where

$$R = \int_{-h}^{0} \phi_0(x)L\{f\}\,\mathrm{d}x + \int_{0}^{h} \phi_1(x)L\{f\}\,\mathrm{d}x. \tag{2.3}$$

Solving for the constants, (2.2) can readily be rewritten in the form

$$\int_{-h}^{h} f(x)\,\mathrm{d}x = (-\lambda^2 B + h)f(-h) + 2\lambda^2 Bf(0) + (-\lambda^2 B + h)f(h) + R, \tag{2.4}$$

where

$$B(1-\cos\lambda h)\lambda^3 = \sin\lambda h - \lambda h\cos\lambda h.$$

Formula (2.4) is now identical to that written in [4] and, for the value $\lambda = 1$ agrees also with that given in [8, p.89]. Later, Vanden Berghe et al. [14] considered generalisations to Ehrenmark's formula essentially by generalising the set $S_3(\lambda)$ to a set $S_n(\lambda)$ with basis $\{1, x, x^2, \dots, x^{n-3}, \sin\lambda x, \cos\lambda x\}$. However, the local truncation error terms were left in integral form for all formulae written therein, although those authors indicated that Ehrenmark's [4] method for determining a closed-form expression for the error term could not be generalised to the higher-order formulae. That closed form can here easily be recovered from (2.3). Moreover, the present method could also be applied in a straightforward manner to the higher-order formulae of Vanden Berghe et al. [14]. Let us define here

$$K(x) = \begin{cases} \phi_0(x), & -h \leqslant x \leqslant 0, \\ \phi_1(x), & 0 \leqslant x \leqslant h, \end{cases} \tag{2.5}$$

so that, provided $\theta \equiv \lambda h < 2\pi$, the graph of $K(x)$ remains similar to that given in [8, p.88] for the "influence function" $\Phi(x)$. It is an odd function of x with zeros at x_0, x_1, x_2 and two turning points. The present form of the remainder term R (i.e., the error) is then given by

$$E[f] \equiv \int_{-h}^{h} K(x)L\{f\}\,\mathrm{d}x \tag{2.6}$$

and the mean value theorem cannot be applied owing to the change of sign of $K(x)$ at $x=0$. Observe however that

$$K^*(x) \equiv \int_{-h}^{x} K(\eta)\,\mathrm{d}\eta$$

is a nonnegative function of x. Integrating (2.6) by parts therefore, we obtain

$$E[f] \equiv -\int_{-h}^{h} K^*(x) L_4\{f\}\,\mathrm{d}x = -L_4\{f\}\Big|_{x=\xi} \int_{-h}^{h} K^*(x)\,\mathrm{d}x, \tag{2.7}$$

where $L_4 \equiv DL_3$, following an application of the mean value theorem. Here $\xi \in [-h, h]$, and carrying out the quadratures, we recover exactly the local truncation error expression as given in [4],

$$k^2 E[f] = -\tfrac{1}{6}h^3 \left\{1 - \frac{6}{\theta}\cot(\theta/2) + 3\cot^2(\theta/2)\right\} L_4\{f\}\Big|_{x=\xi}.$$

3. A five-point rule

A quadrature rule of mixed polynomial and trigonometric type over five points was written in [14] as a special case of a generalised class of formulae. These formulae were characterised by the trigonometric part of the interpolant having a single circular frequency k, as in the above three-point rule. The five-point rule thus studied was denoted a generalised Boole's rule.

Meanwhile, in unpublished work, Rourke [12] had written a new five-point rule based on trigonometric interpolation with two independent frequencies and later, also in unpublished work, Ehrenmark [5] derived an explicit form for the local truncation error of that formula. The formula was simultaneously published in [13] in a form which is a perturbation of the standard Boole's rule. This yields rather unwieldy expressions for the quadrature weights and moreover, as pointed out by those authors, does not readily provide a closed-form expression for the truncation error. In view of this, it is thought prudent to re-present the formula in the light of the technique used above for the three-point rule, since this seems to achieve not only a more symmetrical and easily codeable form for the weights but also the error result in a natural way.

We take the nodes $x_j = (j-2)h$, $j = 0, 1, \ldots, 4$, in conjunction with the operator

$$L_5 \equiv \mathrm{D}(\mathrm{D}^2 + k_1^2)(\mathrm{D}^2 + k_2^2), \quad k_1 \neq k_2.$$

Following the same procedures as before, we can write down a system of subordinate operators required for the extension of Lagrange's identity

$$\begin{aligned} L_4 &= \mathrm{D}^4 + (k_2{}^2 + k_1^2)\mathrm{D}^2 + k_1^2 k_2^2, \\ L_3 &= \mathrm{D}^3 + (k_2{}^2 + k_1^2)\mathrm{D}, \\ L_2 &= \mathrm{D}^2 + (k_2{}^2 + k_1^2), \\ L_1 &= \mathrm{D}, \qquad L_0 = 1. \end{aligned} \tag{3.1}$$

The functions $\phi_i(x)$, $i = 0, \ldots, 3$, have to be chosen to satisfy

$$L_5^* \phi_i(x) = 1$$

having again chosen $w_i = 1$. Expressing the general solution in the form

$$\phi_i(x) = A_i \sin k_1 x + B_i \cos k_1 x + C_i \sin k_2 x + \mathrm{D}_i \cos k_2 x + E_i - \frac{x}{k_1^2 k_2^2},$$

and noting the requirement that the Peano kernel be an odd function, we get the conditions,

$$\begin{aligned}&A_0 = A_3,\ B_0 = -B_3,\ C_0 = C_3,\ D_0 = -D_3,\ E_0 = -E_3,\\ &A_1 = A_2,\ B_1 = -B_2,\ C_1 = C_2,\ D_1 = -D_2,\ E_1 = -E_2.\end{aligned} \tag{3.2}$$

The term for $k=0$ in (2.1) will lead to the quadrature rule itself. The terms for $k=1,\dots,4$ are set equal to zero through the choice of constants. This has to be done independently of the derivatives $f^{(j)}(x_i)$ thus giving us four individual conditions at each of five nodal points

$$\begin{aligned}0 &= \sum_{i=0}^{3} f'(x)L_3^*[\phi_i(x)]\Big|_{x_i}^{x_{i+1}} = \sum_{i=0}^{3} f''(x)L_2^*[\phi_i(x)]\Big|_{x_i}^{x_{i+1}}\\ &= \sum_{i=0}^{3} f^{(3)}(x)L_1^*[\phi_i(x)]\Big|_{x_i}^{x_{i+1}} = \sum_{i=0}^{3} f^{(\mathrm{iv})}(x)\phi_i(x)\Big|_{x_i}^{x_{i+1}}.\end{aligned} \tag{3.2a}$$

The twenty conditions obtained are compatible with system (3.2) and leaves a system for 10 unknown constants, the solution of which is tedious but straightforward. Only the constants E_i are needed to determine the weights in the rule; these are given, along with the full system in Appendix A.

Writing $\theta = k_1 h$ and $\varphi = k_2 h$, it is found that

$$h^{-1}k_1^2k_2^2\Delta^*\{E_0, E_1\} = (1-\cos\varphi)\left(2\cos 2\theta - \frac{\sin 2\theta}{\theta}\right)\{1,\ 1+2\cos\varphi\} - (\theta \leftrightarrow \varphi), \tag{3.3}$$

where

$$\Delta^* \equiv 2(1-\cos\varphi)(1-\cos\theta)(\cos\theta - \cos\varphi). \tag{3.4}$$

In (3.3) and hereafter, $(\theta \leftrightarrow \varphi)$ denotes the entire previous term in the expression with θ and φ interchanged. A simple formula for this five-point rule is then

$$\int_{-2h}^{2h} f(x)\,\mathrm{d}x \approx c_0 f(-2h) + c_1 f(-h) + c_2 f(0) + c_1 f(h) + c_0 f(2h), \tag{3.5}$$

where

$$\begin{aligned}\frac{\Delta^*}{2h}c_0 &= (1-\cos\varphi)\left(1 - \frac{\sin 2\theta}{2\theta}\right) - (\theta \leftrightarrow \varphi),\\ \frac{\Delta^*}{2h}c_1 &= (\cos 2\varphi - 1)\left(1 - \frac{\sin 2\theta}{2\theta}\right) - (\theta \leftrightarrow \varphi),\\ \frac{\Delta^*}{2h}c_2 &= 2\cos\theta(\cos\varphi - \cos 2\varphi)\left(1 - \frac{\sin\theta}{\theta}\right) - (\theta \leftrightarrow \varphi).\end{aligned} \tag{3.6}$$

3.1. Total truncation error

An exact expression for the total truncation error (ltte) is obtained from (2.1). This is

$$E[f] = \int_{-2h}^{2h} K(x) L[f] \, dx, \tag{3.7}$$

where now

$$K(x) = \begin{cases} \phi_0(x), & -2h \leqslant x < -h, \\ \phi_1(x), & -h \leqslant x \leqslant 0. \end{cases}$$

$L \equiv L_5$ and $K(x)$ is defined in $[0, 2h]$ by $K(x) = -K(-x)$. Using the earlier procedure, we define

$$K^*(x) = \int_{-2h}^{x} K(\eta) \, d\eta \tag{3.8}$$

and noting also that $K^*(2h) = 0$, an integration by parts yields

$$E[f] = -\int_{-2h}^{2h} K^*(x) \, \mathrm{D}L[f] \, dx. \tag{3.9}$$

We will now assume, without loss of generality, that $\varphi > \theta$. Note that the case $\varphi = \theta$ is degenerate and will lead to a second generalised Boole's rule. This is fully discussed in Section 6. We require that $K^*(x)$ be of one sign on $[-2h, 2h]$. The positivity of K of course implies that of K^* on $]-2h, 2h[$. It is easy to see that, as φ increases, a first zero of K develops near $x = -2h$, for some critical value φ_{crit} of φ, with the result that K^* synchronously develops a zero. The validity of a Mean Value Theorem application then requires $\varphi < \varphi_{\text{crit}}$.

It is established in Appendix B that ϕ_0 remains of one sign on the interval $[-2h, -h]$ provided $\varphi^2 < 3$. A slightly weaker result is established for ϕ_1 on $[-h, 0]$ so that $K(\eta)$ remains of one sign at least on $[-2h, 0]$ and also, by its parity, on $[0, 2h]$ provided $0 < \theta < \varphi \leqslant 0.43$. The essential part, of course, is that the interval is *independent of h.*

Following the assumption above, the explicit form for the local truncation error is now readily obtained by application of the mean value theorem to Eq. (4.8). We have

$$E[f] = -\mathrm{D}L[f]|_{x=\xi} \int_{-2h}^{2h} K^*(x) \, dx.$$

Either by completing the quadrature, or by applying this result and the quadrature rule itself to $f \equiv x^2$, we obtain finally

$$E[f] = -\mathrm{D}L[f]|_{x=\xi} \frac{h^6}{\theta^2 \varphi^2} \left[4c_0 + c_1 - \frac{8h}{3} \right]. \tag{3.10}$$

It may be verified that this reduces, in the limits $\theta, \varphi \to 0$, to the well-known error of the Newton–Cotes five-point (Boole's) rule, namely $-\frac{8}{945} h^7 f^{(6)}(\xi)$.

4. Optimisation strategies

In the earliest application of formula (2.4) [4] the parameter k was chosen by various methods ranging from prescriptive constant, linear and logarithmic variation to an "on-line" method where its choice was updated as appropriate simply by automated observation of local wave frequency through tracking the change of sign of the integrand as integration proceeded. These early ideas were improved in [13], which introduced the idea of choosing k by minimising $-\mathrm{D}L[f]|_{x=\xi}$. It was thought that the (local) choice, where $\xi = \eta$ was to be the mid-point of each subinterval of integration, would in general give a smaller value of the (global) error than any other particular choice and this was backed up with numerical evidence to confirm the idea.

This idea was also pursued in the work [13] that first published the present five-point rule. Those authors noted the proportionality only, of the ltte to the quantity$-\mathrm{D}L[f]|_{x=\eta}$ where, from now, L is the operator L_5 as defined in Section 3. They also noted that, in addition to the equation $-\mathrm{D}L[f]|_{x=\text{mid-point}} = 0$, a second equation was required fully to determine usable pairs of values for k_1, k_2. Their approach was to expand the first condition in a series about the mid-point of the panel and use the dominant part of this as the second condition: $-\mathrm{D}^2L[f]|_{x=\text{mid-point}} = 0$. The authors had to conclude, however, that numerical results from this procedure were somewhat disappointing. They reported possible stability problems and suggested the remedy of using instead $-\mathrm{D}^3L[f]|_{x=\text{mid-point}} = 0$. Although still only a locally determined strategy, they now found a significant improvement in the numerical results obtained in two examples that had been earlier studied elsewhere. Some further discussion of their results are presented in Section 5.

More recently, Köhler [10], in discussing the errors in a class of formulae which does not include the present five-point rule, introduces a strategy of minimising the *global error* in a computation over N panels of width H by, if so desired, a single choice of the parameter. Quoted here is Theorem 1.1 of Köhler [10] retaining the notation therein:

$$R_N[f] = H^{r+1}\sum_{j=0}^{k} H^j \int_a^b \mathrm{D}^{j+1}\{\mathrm{D}^r + \lambda^2\mathrm{D}^{r-2}\}f(x)\,\mathrm{d}x \sum_{\mu=0}^{\infty} \eta_{\mu,j}(\lambda H)^\mu + \mathrm{O}(H^{r+2+k}), \tag{4.1}$$

where, purely for convenience, r is here taken odd. In this, $\eta_{\mu,j}$ depend only on r and $\eta_{\mu,j} = 0$ if either μ or j is odd. In the case of the three-point formula ($r = 3$), for example, the choice

$$\int_a^b \mathrm{D}\{\mathrm{D}^3 + \lambda^2\mathrm{D}\}f(x)\,\mathrm{d}x = 0 \tag{4.2}$$

may be attempted, with the result that $R_N[f] = \mathrm{O}(H^6)$. Köhler notes that this strategy may, or may not work, depending on whether, or not, it happens that $f'(b) = f'(a)$, but several examples are given to indicate the considerable strength of this method. If we look at the next term of $R_N[f]$ above, it is easily seen to be proportional to $\int_a^b \mathrm{D}^3\{\mathrm{D}^3 + \lambda^2\mathrm{D}\}f(x)\,\mathrm{d}x$.

The question then arises of extending the Köhler theory to the present fifth-order operator. In the sense of Köhler's analysis [10], L_5 does not belong to the set of operators $\mathrm{D}_{r,\lambda}$ considered there, these depending only on one single-parameter λ in any one (subinterval) application. We present instead here, an ad hoc proof that, essentially the same arguments on the optimisation of global error may indeed be used for the operator L_5 which has two free parameters and moreover this focus on L_5 will give us a closed-form estimate of the global error term.

First note smoothness properties of $K^*(\eta)$. From the conditions extracted by (3.2) and (3.2a) it follows that $K \in C^3(-2h, 2h)$ and consequently that $K^* \in C^4(-2h, 2h)$. Now let $\tilde{K}^*$ be the periodic extension of K^* onto the whole interval of integration $[a, b]$ where it will be assumed (purely for convenience) that the interval is covered by an odd number of panels of width $H = 4h$. Thus, the mid-point $x_m = (a+b)/2$ is a mid-point of a panel. Since ϕ_0 has a quadruple zero at $x = -2h$, it follows that $\tilde{K}^*$ has zeros of order 5 at each panel end-point. Thus, $\tilde{K}^* \in C^4(a, b)$.

Let the global error in a composite application of (3.5) over $[a, b]$ be given by $E_\sigma[f]$. (We deliberately avoid Köhler's [10] notation $R_N[f]$ to distinguish). From (3.9) there follows

$$E_\sigma[f] = -\int_a^b \tilde{K}^*(x)\mathrm{D}L[f]\,\mathrm{d}x. \tag{4.3}$$

Now make the further definition

$$\hat{K}(x) = \int_{x_m}^{x} \tilde{K}^*(\eta)\,\mathrm{d}\eta, \tag{4.4}$$

so that, after an integration by parts of (4.3), we have

$$E_\sigma[f] = \int_a^b \hat{K}(x)\mathrm{D}^2L[f]\,\mathrm{d}x - \hat{K}(b)\{\mathrm{D}L[f]|_a + \mathrm{D}L[f]|_b\} \tag{4.5}$$

since $\hat{K}(x)$ is *odd* about $x = x_m$. Next, define the constant μ by $\mu(b - x_m) = \hat{K}(b)$ and let

$$\Lambda \equiv \int_a^b \mu(x - x_m)\mathrm{D}^2L[f]\,\mathrm{d}x. \tag{4.6}$$

Then if, after [10], we choose

$$\int_a^b \mathrm{D}L[f]\,\mathrm{d}x = 0, \tag{4.7}$$

it follows upon integrating also (4.6) by parts, that

$$\Lambda = \frac{\mu(b-a)}{2}\{\mathrm{D}L[f]|_a + \mathrm{D}L[f]|_b\}.$$

In view of the above, (4.5) now simplifies to

$$E_\sigma[f] = \int_a^b \{\hat{K}(x) - \mu(x - x_m)\}\mathrm{D}^2L[f]\,\mathrm{d}x, \tag{4.8}$$

where it may be observed that $\hat{K}(x)$ coincides with $\mu(x - x_m)$ at each panel end-point. Now consider the further choice (if possible)

$$\int_a^b \mathrm{D}^3L[f]\,\mathrm{d}x = 0. \tag{4.9}$$

We continue by writing

$$\tilde{L}_1(x) = \int_{x_m}^{x} \{\hat{K}(x) - \mu(x - x_m)\}\,\mathrm{d}x \tag{4.10}$$

so that, following a further integration by parts of (4.8), we obtain

$$E_\sigma[f] = -\int_a^b \tilde{L}_1(x) \mathrm{D}^3 L[f]\,\mathrm{d}x, \tag{4.11}$$

since $\tilde{L}_1(x)$ is symmetric about $x = x_m$. Note that we have yet to exploit (4.9). We can repeat the manipulation which transformed (4.3) into (4.8). This involves writing further,

$$\tilde{L}_2(x) = \int_{x_m}^{x} \tilde{L}_1(x)\,\mathrm{d}x, \qquad \tilde{L}_2(b) = \lambda(b - x_m), \qquad \tilde{L}_3(x) = \int_{x_m}^{x} \{\tilde{L}_2 - \lambda(x - x_m)\}\,\mathrm{d}x$$

so that after another integration by parts and now making use of (4.9),

$$E_\sigma[f] = \int_a^b \{\tilde{L}_2 - \lambda(x - x_m)\} \mathrm{D}^4 L[f]\,\mathrm{d}x. \tag{4.12}$$

Integrating one final time and noting the even symmetry of L_3 about x_m, we arrive at a theorem.

Theorem. *Let* $f \in C^{10}[a,b]$. *Let* $(b-a) = NH$, $H = 4h$, $(N+1)/2 \in \mathbb{N}$ *and let* E_σ *be defined by* $E_\sigma[f] \equiv \int_a^b \tilde{K}_h(x) L[f]\,\mathrm{d}x$, *where* $\tilde{K}_h$ *is the* $4h$-periodic *extension of* K *defined by* (3.7 *et seq.*) *and where* $L \equiv \mathrm{D}(\mathrm{D}^2 + k_1^2)(\mathrm{D}^2 + k_2^2)$, $k_1, k_2 \in \mathbb{R}$. *Then, if* k_1, k_2 *can be chosen such that*

$$\int_a^b \mathrm{D}L[f]\,\mathrm{d}x = \int_a^b \mathrm{D}^3 L[f]\,\mathrm{d}x = 0,$$

it follows that

$$E_\sigma[f] = \tilde{L}_3(b) \mathrm{D}^4 L[f]|_a^b - \int_a^b \tilde{L}_3(x) \mathrm{D}^5 L[f]\mathrm{d}x. \tag{4.13}$$

Remark 1. For values of θ, ϕ $(0 < \theta < \varphi \leqslant 0.43)$ for which the Peano kernel K remains of one sign in each half interval $[-2h, 0], [0, 2h]$ (see Appendix B), it follows that K^* is monotonic increasing in $[-2h, 0]$ and symmetric about $x = 0$. Since the behaviour of K^* near $x = \pm 2h$ is like that of $Q(x \mp 2h)^5$, for some constant Q, it also follows by symmetry, not only that $\hat{K} - \mu(x - x_m)$ is periodic with period of a panel width, vanishes at the mid-point of every panel of quadrature and has odd symmetry about such a point, but also, with $\hat{K}$ increasing, that $\hat{K} - \mu(x - x_m)$ is negative in the r.h. half of every panel. Thus, $\tilde{L}_1$ is similarly periodic and *negative definite*. Clearly, the same conclusions are drawn for $\tilde{L}_3$.

Remark 2. In view of Remark 1, we can now estimate also the integral term in (4.13), using the mean value theorem in the usual way. We get

$$E_\sigma[f] = \tilde{L}_3(b) \mathrm{D}^4 L[f]|_a^b - \mathrm{D}^5 L[f]|_{x=\xi} \int_a^b \tilde{L}_3(x)\,\mathrm{d}x. \tag{4.13a}$$

Remark 3. $\tilde{L}_3(b)$ and $\int_a^b \tilde{L}_3(x)\,\mathrm{d}x$ can be formally evaluated by the several quadratures following the specification of K in (3.7 *et seq.*). The above result is chiefly of interest in establishing the role of (4.7) and (4.9) in determining an error reduction of $O(h^4)$, we get however

$$\tilde{L}_3(b) = \int_0^{2h} K(t) \left\{ \frac{t^4}{4!} - \frac{h\,t^3}{3!} + \frac{h^3 t}{3} \right\} \mathrm{d}t;$$

$$\int_0^{2h} \tilde{L}_3(x)\mathrm{d}x = -\int_0^{2h} K(t) \left\{ \frac{t^5}{5!} - \frac{2ht^4}{4!} + \frac{4h^2 t^3}{3.3!} - \frac{16h^4 t}{45} \right\} \mathrm{d}t.$$

It is perhaps of interest to note the asymptotic forms of these as $h \to 0$, although the reader trying to relate these to similar expressions from conventional Newton–Cotes rules will need to remember that k_1, k_2 have now been fixed by Eqs. (4.7) and (4.9) so that it is not possible to replace, for example, $D^4 L[f]$ by D^9 in this limit. After some further computations (detailed in Appendix C), we obtain,

$$\tilde{L}_3(b) \sim -124h^{10}/127\,575; \qquad \int_0^{2h} \tilde{L}_3(x)\,\mathrm{d}x \sim -5557h^{11}/5\,613\,300.$$

Some remarks relating to the global error term are made in connection with Example 2 in the next section.

5. Numerical implications

We have two conditions, (4.7) and (4.12), to satisfy in order to optimise the global error. Both of these are of the fundamental type

$$A + B(k_1^2 + k_2^2) + C\,k_1^2 k_2^2 = 0, \tag{5.1}$$

regarded as curves in the (phase) space (k_1, k_2). The ideal situation is that these curves, called "error curves" in some of the diagrams below, intersect in an easily identifiable point which will determine the parameter values for the integration routine and the error estimate (4.13) becomes applicable (in practice only to indicate the order of magnitude). Two examples are presented to illustrate this. In these, and others that follow, the curves C_1 and C_2 are (5.1) with the respective choices:

$$A = (D^5 f)|_a^b, \quad B = (D^3 f)|_a^b, \quad C = (Df)|_a^b$$

and

$$A = (D^7 f)|_a^b, \quad B = (D^5 f)|_a^b, \quad C = (D^3 f)|_a^b.$$

Example 1.

$$\int_0^{2\pi} x \sin 20x \cos 50x \,\mathrm{d}x.$$

This example was tested e.g. in [4] for the three-point rule and in [5] for the five-point rule. Van Daele et al. [5] explained why it works rather better than it deserves to for the choice $k_1 = 30$, $k_2 = 70$ (which are exact solutions to the optimisation constraints). Nevertheless, it is an excellent example to demonstrate the technique of choosing optimum (k_1,k_2) as described here. Thus, Fig. 1 shows the two curves computed by two methods; firstly by exact differentiation (using a symbolic differentiation package) and secondly by use of finite difference operators to estimate the derivatives at end points a and b. There is virtually no detectable difference on the diagrams, the curves in each case intersecting, as predicted, at (30,70) and (70,30).

Remark (i). The modified example where the polynomial x is replaced by x^2 showed an identical behaviour with $k_1 = 30$, $k_2 = 70$ being optimum values.

Remark (ii). The instability referred to in [13] in *local* applications is more than likely related to the relative ill-conditioning of systems like $\int_a^b \mathrm{D}L[f]\mathrm{d}x = \int_a^b \mathrm{D}^3L[f]\mathrm{d}x = 0$, which is likely to be enhanced when $\mathrm{D}^3 \to \mathrm{D}^2$, as was the case in [13]. This element of ill-conditioning is visually evident in Fig. 1.

Example 2.

$$\int_0^{2\pi} x^2 (\sin 20x + \cos 50x)\,\mathrm{d}x = \frac{1}{5}\pi\left(\frac{1}{125} - \pi\right)$$

The two error curves intersect at points in $\mathbb{R}^2$ for this example also. The curves are shown in Fig. 2 and one point of intersection $(k_1,k_2)^{(0)} = (19.401, 58.067)$. For this example, we have also computed the error in calculation over a rectangular domain $(k_1,k_2) \in [1, 80] \times [1, 80]$. The results of this computation which represent an impressive vindication of the theory provided are displayed (inset) in the same diagram. This error computation was done with $N = 100$. The opportunity was also taken of "examining" the global error term (4.13a). The error $1.2 \cdot 10^{-10}$ was computed for $N = 200$ using the optimal k-values and $-2.1816 \cdot 10^{-7}$ was obtained in an exact calculation of $\mathrm{D}^4L[f]|_a^b h^{10}$. The first term of (4.13a) is therefore $2.12 \cdot 10^{-10}$ making the actual error less and of the right order of magnitude. It is not possible to be more specific in view of the uncertainty of the second term involving $\mathrm{D}^5L[f]$. Moreover, comparison with the error $2 \cdot 10^{-7}$, obtained with $N = 100$ shows the asymptotic dependence $\mathrm{O}(h^{10})$ to be accurate allowing for the small oscillations in error as h is varied.

Remark (iii). The error at $(k_1,k_2)^{(0)}$ is of course not an actual minimum. In many of these cases the "global error surface" will cut the (k_1,k_2) plane and there will be a "zero error curve". If the two error curves C_1, C_2 do not intersect, we can expect the zero error curve to lie in the space between C_1 and C_2. The reason for this can be seen intuitively from Köhler's expansion (4.1) herein, where, if f is sufficiently oscillatory, $\mathrm{D}^n f$ and $\mathrm{D}^{n+2} f$ are clearly of opposite sign. Thus, the dominant "error surface" inclines downwards if its first "correction" is inclined upwards (and vice versa). However, without further analysis of the type described in Section 4, it would not be possible to get closer to this curve in general, except by pure chance. On the other hand, it may be that some extrapolative techniques could be used to trap the position of the zero error curve more closely. Further work on this could be worthwhile. The next example illustrates the phenomenon.

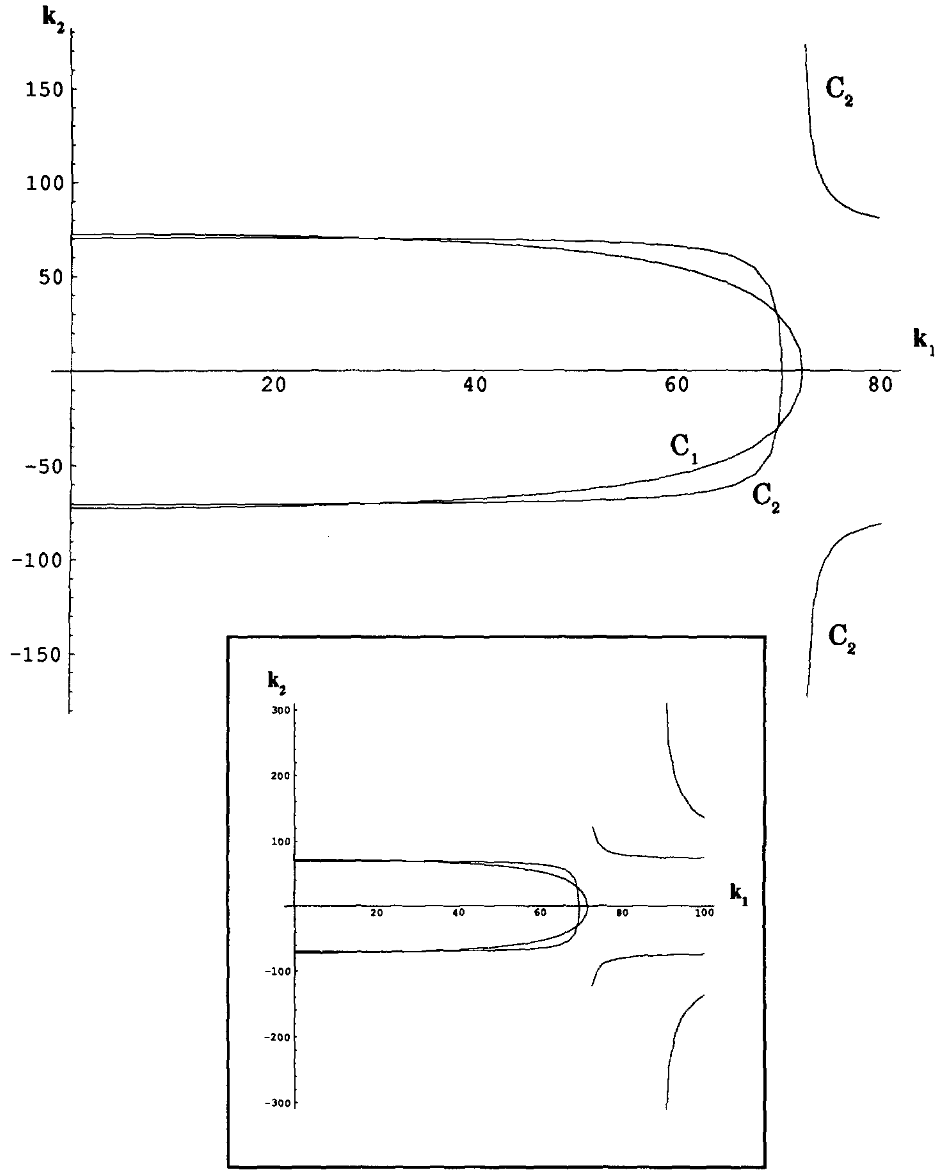

Fig. 1. Graphs showing optimum error curves (Eq. 4.7: C_1 and 4.12: C_2) for Example 1:

$$\int_0^{2\pi} x \sin 20x \cos 50x \, dx$$

Main graph is exact computation. Inset graph obtained by finite differences approximations.

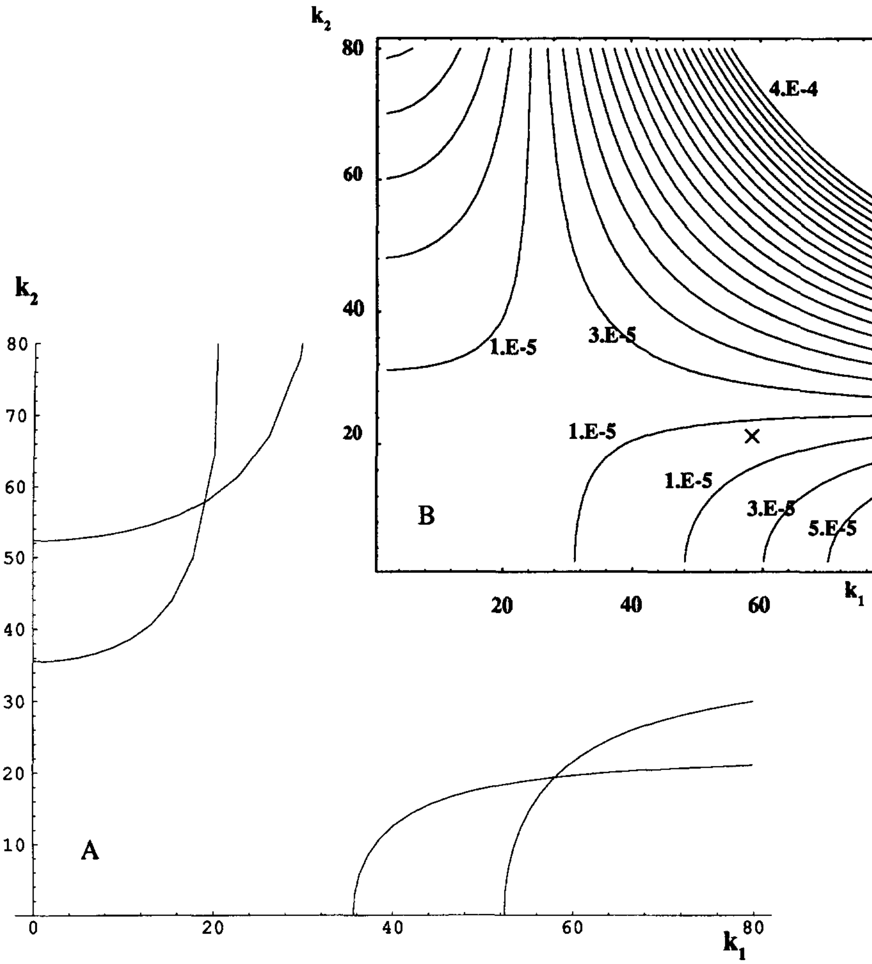

Fig. 2. Main Graph (A) shows the two optimising error curves (Eqs. 4.7 and 4.12) for computation in Example 2. Upper (inset) graph is a contour plot of the actual absolute errors. Note that intersection of curves in A is indicated by the cross in **B** and lies in the valley represented by the domain of minimum error. Error at this point $(19.40, 58.01) = 2.\mathrm{E}-7$.

Example 3.

$$\int_0^{2\pi} x^2 \sin x \sin 20x \cos 50x \, dx = \pi \left\{ \tfrac{1}{69^2} - \tfrac{1}{71^2} - \tfrac{1}{29^2} + \tfrac{1}{31^2} \right\}.$$

The two optimising error curves for this example are shown in Fig. 3. The curves do not intersect in the $\mathbb{R}^2$ plane. However, the computation of points for which the absolute error is less than 1.d-11 (with $N = 200$) was undertaken independently and the aggregate of these points (shown only for $k_2 > k_1$) are plotted. It is seen that this aggregate is exactly as predicted above.

Although there is no intersection in $\mathbb{R}^2$, Eqs. (4.7) and (4.12) remain soluble for complex values and we get $k_1 = 128.952 + 58.824i$, $k_2 = \bar{k}_1$. To examine the structure of the true error surface in the

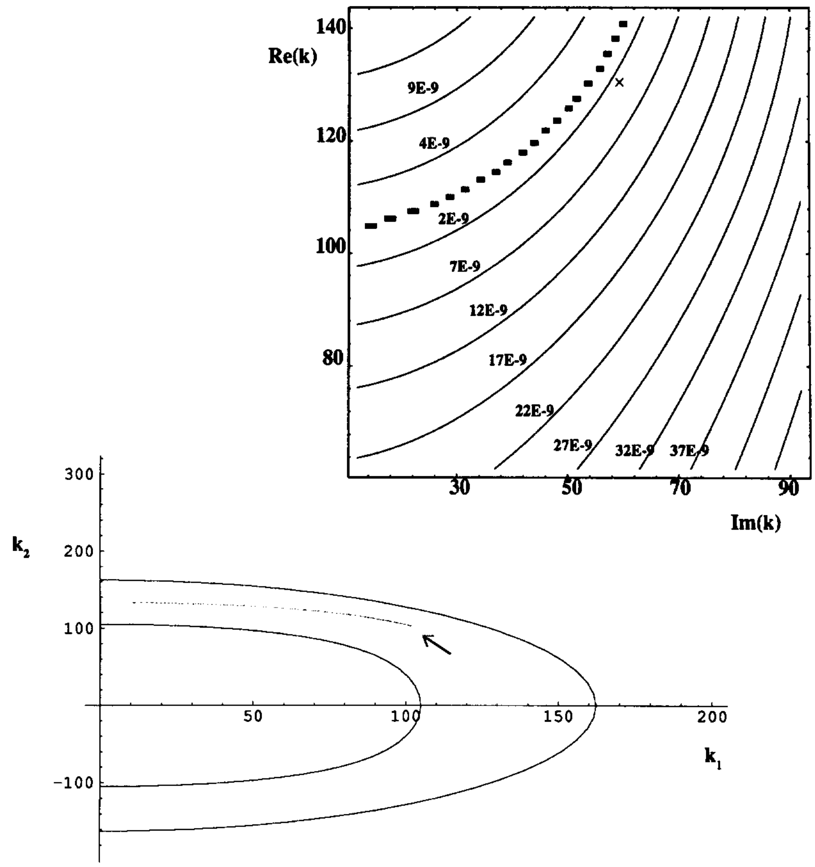

Fig. 3. *Lower Graph* shows optimum error curves (Eqs. 4.7 and 4.12) for the quadrature of Example 2:

$$\int_0^{2\pi} x^2 \sin x \sin 20x \cos 50x \, dx$$

Note points plotted (arrowed) represent values of parameters for which absolute error calculated (with $k_2 > k_1$ and $N=200$) is less than 1.d−11. *Upper Graph* shows contours of actual absolute errors for computations with complex conjugate values of parameters. Thick dashed line indicates approximately bottom of the 'valley'. Note position of cross: Corresponds to complex intersection of error curves in lower graph.

vicinity of such a point, a map is also shown giving contours of the absolute error for a range of values of real and imaginary k_1. The proximity of the given point to the bottom of the error surface valley is considered quite remarkable.

Example 4.

$$\int_0^{2\pi} x^2 \sin x^3 \, dx = (1 - \cos 8\pi^3)/3.$$

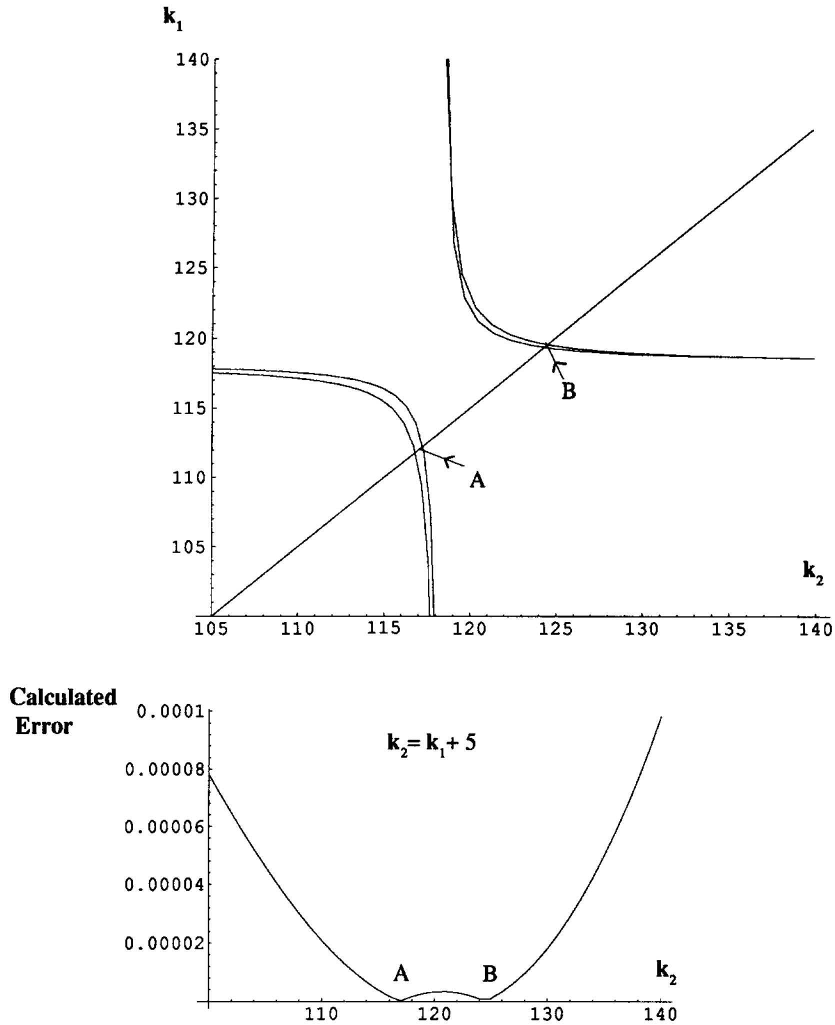

Fig. 4. Upper graph shows optimum error curves for Example 4. Lower graph shows actual errors computed on Section $k_2 = k_1 + 5$. Note that section is shown by straight line in upper graph. Shown also in that graph are points A and B representing the minimum errors in the lower graph.

$$A: k_2 = 117$$
$$B: k_2 = 124.5$$

This example was chosen to illustrate that the method works equally well for functions with a strongly varying frequency. Results are shown in Fig. 4 where it is seen that, whereas the primary branches of the error curves do not cut in $\mathbb{R}^2$, the secondary branches do. The cuts are at $(k_1, k_2) = (118.625, 137.705)$ (or $(k_1 \leftrightarrow k_2)$). By looking carefully at the distribution of actual calculated absolute error, we can see again that, between the two primary branches of the curves, there are positions of zero error. A reasonable way to illustrate this is by a simple section of the error surface. Here, the cut $k_1 + 5 = k_2$ is shown and two points A (primary) and B (secondary) are indicated where the error is locally minimised. These two points sit very accurately between the appropriate parts of the error curves. It is noted that the "valley" at B is not at zero, whereas that at A is at zero by virtue of the signed error changing sign at A. The error computation was done with $N = 200$.

6. Concluding remarks and a new generalised Boole's rule

Both local and global truncation errors have been established, in closed form, for the generalised five-point quadrature formula with two free parameters, first published in [13]. Moreover, a theorem has been proved, which shows that earlier work in [10] on the optimisation of error for a different class of rules may be extended (at least in part) also to the present rule. Thus, it has been demonstrated that, in certain circumstances, a pair of curves exist in the parameter space such that their intersection represents, in general, a reduction in global error of order h^4. Furthermore, it has been shown by examples, that where no intersection of the curves takes place for real values of the parameters, a pair of complex conjugate values will yield a similar reduction in error.

There is one further simple example that is worthy of consideration.

Example 5.

$$\int_{0.1}^{\pi} x(3\cos 3x \cos 17x - 17 \sin 3x \sin 17x)\,\mathrm{d}x = 0.9567255461112044D - 4.$$

The error curves are shown in Fig. 5, from which it is clear that the proposed formula could operate best if we choose $k_1 = k_2 \approx 21\ldots$. This is not possible in the present formulation since we have the restriction $k_1 < k_2$. Our five-point formula is degenerate if the parameters are chosen equal. Let us therefore examine the limit $k_1 \to k_2$, without either being small.

From Eqs. (3.4) and (3.6), and writing $c^{(j)} = \mathrm{Lim}_{k_1 \to k_2} c_j$, there follows

$$\{c^{(0)}, c^{(1)}\} = \frac{h}{(1-\cos\theta)^2}\{S - (1-\cos\theta)C, \qquad -4S\cos\theta + (1-\cos 2\theta)C\}, \tag{6.1}$$

where

$$S \equiv \left(1 - \frac{\sin 2\theta}{2\theta}\right), \qquad C \equiv \left(\frac{\cos\theta}{\theta^2} - \frac{\cos 2\theta}{\theta \sin\theta}\right). \tag{6.2}$$

The remaining constant $c^{(2)}$ is determined by

$$c^{(0)} + c^{(1)} + \tfrac{1}{2}c^{(2)} = 2h. \tag{6.3}$$

We have thereby written a further, single parameter, five-point rule which may be contrasted with the five-point generalisation to Boole's rule first given in [13]. The application of the new rule (with $N = 110$) to the example above, gives the relative error -1×10^{-10} when the free parameter k is given the value 20.293 chosen by setting $k_1 = k_2$ in (4.7).

We conclude with a comparison between the new and the old generalisations to Boole's rule. The old rule as proposed in [14], integrates exactly any combination from the set $\{1, x, x^2, \sin kx, \cos kx\}$.

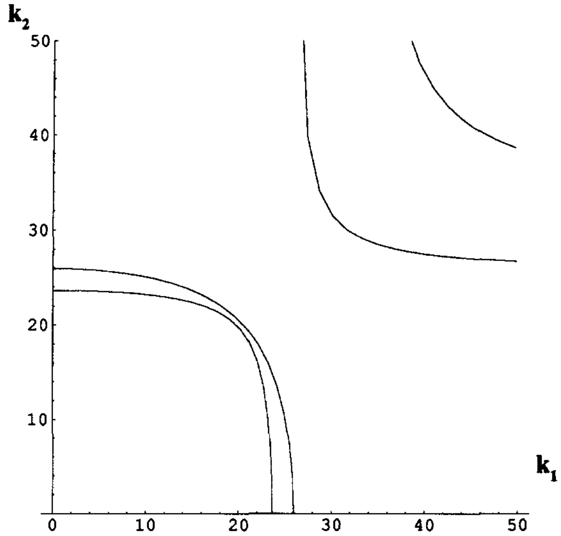

Fig. 5. Error curves for the quadrature of Example 5. Note close contact of principal branches at $k_1 = k_2$.

It is convenient to rewrite the coefficients for that quadrature to the form used in the present work. With the obvious notation, we have

$$c_0|_{\mathrm{Old}} = \frac{h}{(1-\cos\theta)^2}\left\{\frac{4}{3}(1-\cos\theta) - \left(1 - \frac{\sin 2\theta}{2\theta}\right)\right\},$$

$$c_1|_{\mathrm{Old}} = \frac{-4h}{(1-\cos\theta)^2}\left\{\frac{1}{3}(1-\cos 2\theta) - \left(1 - \frac{\sin 2\theta}{2\theta}\right)\right\}$$

and $c_2|_{\mathrm{Old}}$ may be determined as in (6.3) using $\{c_0, c_1\}|_{\mathrm{Old}}$.

The new rule, proposed here in Eqs. (6.1)–(6.3) integrates exactly any combination from the set $\{1, \sin kx, \cos kx, x\sin kx, x\cos kx\}$. In order to make the comparison fair, the above example is computed using these two rules both with constant values of the parameter k but specified, in each case, by Köhler's technique using the two respective operators $L_{\mathrm{Old}} \equiv \mathrm{D}^3(\mathrm{D}^2 + k^2)$ and $L_{\mathrm{new}} \equiv \mathrm{D}(\mathrm{D}^2 + k^2)^2$. The results are shown in Table 1, with the new rule having a distinct advantage over the old rule.

The opportunity is also taken of comparing the results obtained in this way with those obtained originally in [14] where the parameter k was varied locally in each subinterval. Those authors, in considering Example 1 of the present text, obtained a relative error $O(2 \times 10^{-6})$ with 110 (N) functional evaluations over the interval. Keeping the same number of evaluations (i.e., same step length h) we record a striking improvement using Köhler's method. This improvement is recorded for both cases when k_{opt} is computed either by finite differences or by an exact analytic method. The functional evaluations to do the former are basically insignificant since they are done just once, instead of at each subinterval as in [14]. The results are shown in Table 2. It should also be remarked, in passing, that the method in the latter paper seems to be quite unstable. Those authors have themselves remarked that negative values of k^2 can be anticipated and that, in such

Table 1
Computation (using $N = 110$) of integral in Example 5, with the parameter k optimised using finite difference approximation to Köhler's rule

Parameter k	Relative errors
New generalised Boole's rule:	
20.892	$-1.09 \cdot 10^{-10}$
20.692	$-1.07 \cdot 10^{-10}$
20.492	$-1.04 \cdot 10^{-10}$
20.292	$\mathbf{-1.03 \cdot 10^{-10}}$
20.092	$-1.01 \cdot 10^{-10}$
19.892	$-9.89 \cdot 10^{-11}$
19.692	$-9.68 \cdot 10^{-11}$
19.492	$-9.46 \cdot 10^{-11}$
Old generalised Boole's rule:	
26.534	$-0.28 \cdot 10^{-7}$
26.334	$-0.19 \cdot 10^{-7}$
26.134	$-0.10 \cdot 10^{-7}$
25.934	$\mathbf{-0.19 \cdot 10^{-8}}$
25.734	$0.67 \cdot 10^{-8}$
25.534	$0.15 \cdot 10^{-7}$
25.334	$0.24 \cdot 10^{-7}$
25.134	$0.32 \cdot 10^{-7}$

Note: (i) Optimised value is shown in bold. (ii) The parameter value is determined by F/D approximation.

Table 2
Computation (using $N = 110$) of integral in Example 1

Parameter k	Relative errors
New generalised Boole's rule:	
58.19	$-8.06 \cdot 10^{-9}$
57.99	$-4.53 \cdot 10^{-9}$
57.79	$-9.92 \cdot 10^{-10}$
57.59	$2.55 \cdot 10^{-9}$
57.391	$\mathbf{6.10 \cdot 10^{-9}}$
57.19	$9.66 \cdot 10^{-9}$
56.99	$1.32 \cdot 10^{-8}$
56.79	$1.68 \cdot 10^{-8}$
56.59	$2.03 \cdot 10^{-8}$

Note: (i) The Optimum parameter value determined exactly: $k = 57.4456$. (ii) The parameter value determined by F/D approximation is shown in bold.

intervals, the quadrature weights have to be changed to their hyberbolic counterparts. The graph in Fig. 6 shows a plot of their definition of k^2 for this example. Clearly, only very careful selection of either the number of subintervals, or the point in a subinterval at which k is computed, will avoid

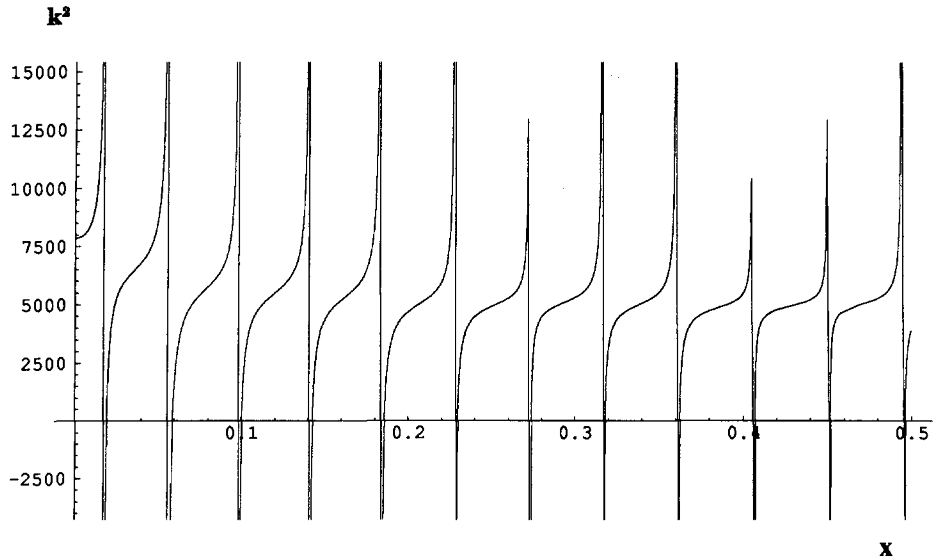

Fig. 6. Graph of parameter k^2 where k is defined by

$$k = \left[\frac{f^{(6)}(x)}{f^{(4)}(x)}\right]$$

for integral of Example 1

negative values of k^2 and the double coding routine implied by this that would be necessary in most applications. These negative values are the result of some local interference between the oscillatory components of the integrand. The global strategy will of course in general avoid the problem.

Acknowledgements

The author wishes to record sincere thanks to an anonymous referee whose thorough work on an earlier draft led to a significant error being detected and a number of additional small improvements made.

Appendix A

We write the 10 relations from which the constants determining ϕ_0, ϕ_1 may be found. Four conditions are obtained at $x = -2h$, namely

$$A_0 \sin 2\theta - B_0 \cos 2\theta + C_0 \sin 2\varphi - D_0 \cos 2\varphi = E_0 + 2h/k_1^2 k_2^2,$$

$$\theta(A_0 \cos 2\theta + B_0 \sin 2\theta) + \varphi(C_0 \cos 2\varphi + D_0 \sin 2\varphi) = h/k_1^2 k_2^2,$$

$$\varphi^2(A_0 \sin 2\theta - B_0 \cos 2\theta) + \theta^2(C_0 \sin 2\varphi - D_0 \cos 2\varphi)$$

$$= (\theta^2 + \varphi^2)E_0 + 2h^3(k_1^2 + k_2^2)/k_1^2k_2^2,$$

$$\theta\varphi^2(A_0 \cos 2\theta + B_0 \sin 2\theta) + \varphi\theta^2(C_0 \cos 2\varphi + D_0 \sin 2\varphi) = h^3(k_1^2 + k_2^2)/k_1^2k_2^2.$$

Likewise, the four conditions at $x = -h$ are

$$A_2 \sin\theta + B_2 \cos\theta + C_2 \sin\varphi + D_2 \cos\varphi + E_2$$
$$= A_3 \sin\theta + B_3 \cos\theta + C_3 \sin\varphi + D_3 \cos\varphi + E_3,$$

$$\theta(A_2 \cos\theta - B_2 \sin\theta) + \varphi(C_2 \cos\varphi - D_2 \sin\varphi)$$
$$= \theta(A_3 \cos\theta - B_3 \sin\theta) + \varphi(C_3 \cos\varphi - D_3 \sin\varphi),$$

$$\varphi^2(A_2 \sin\theta + B_2 \cos\theta) + \theta^2(C_2 \sin\varphi + D_2 \cos\varphi) + (\theta^2 + \varphi^2)E_2$$
$$= \varphi^2(A_3 \sin\theta + B_3 \cos\theta) + \theta^2(C_3 \sin\varphi + D_3 \cos\varphi) + (\theta^2 + \varphi^2)E_3,$$

and

$$\varphi(A_2 \cos\theta - B_2 \sin\theta) + \theta(C_2 \cos\varphi - D_2 \sin\varphi)$$
$$= \varphi(A_3 \cos\theta - B_3 \sin\theta) + \theta(C_3 \cos\varphi - D_3 \sin\varphi).$$

The eight conditions at $x = h$ and $x = 2h$ are automatically satisfied by the parity conditions as are two of the conditions at $x = 0$. The remaining two there are

$$B_1 + D_1 + E_1 = 0$$

and

$$k_2^2B_1 + k_1^2D_1 + (k_1^2 + k_2^2)E_1 = 0.$$

In the interest of brevity, we write (in Section 4) only the solutions for E_0, E_1. Other quantities are then easily determined by backsubstitution.

Appendix B

We need to establish conditions on θ, φ which will be sufficient to protect the kernel K from a change of sign in the interval $[-2h, -h]$. This, in order that the M.V.T. may be applied to determine a closed form for the total truncation error. Here $K = \phi_0(x)$ and from the conditions given in Appendix A, it is straightforward to show that ϕ_0 has a quadruple zero at $x = -2h$. Writing $M_4 = \phi_0^{(\mathrm{iv})}(-2h)$, we can write a Taylor expansion of ϕ_0 about this point, thus

$$\phi_0(-2h + \xi) = M_4 \sum_{k=2}^{\infty} \frac{(-1)^k}{(2k)!} \xi^{2k} \left\{ \frac{k_2^{2k-2} - k_1^{2k-2}}{k_2^2 - k_1^2} \right\} + \xi \sum_{k=2}^{\infty} \frac{(-1)^{k+1}}{(2k+1)!} \xi^{2k} \left\{ \frac{k_2^{2k-2} - k_1^{2k-2}}{k_2^2 - k_1^2} \right\}.$$

The procedure adopted is to isolate the first three terms of the above in ascending powers of ξ. The remaining expansion can then be taken in pairs of terms with each pair being a positive quantity. In this way we can deduce a minimum bound for the first zero of ϕ_0 greater than $-2h$ by determining the zero of the three-term expansion – the same technique applied to, for example, the Maclaurin expansion for $\sin x$ yields the lower bound $\sqrt{6}$ for the zero at π.

The positivity of the tail follows from the assertion that

$$1 > \frac{\xi^2 k_2^2}{(4N+4)(4N+5)} \left\{ \frac{1-\sigma^{4N+2}}{1-\sigma^{4N}} \right\}, \quad \sigma = \frac{k_1}{k_2} < 1, \ N = 1,2,\ldots$$

which, since $\xi \in [0,h]$, can be guaranteed by the restriction $\varphi^2 < 36$. Meanwhile, the relevant zero of the three-term expansion is given by

$$\xi_0 = \frac{3}{M_4(k_2^2+k_1^2)} \{ (1 + \tfrac{10}{3} M_4^2 (k_2^2 + k_1^2))^{\frac{1}{2}} - 1 \}. \tag{B.1}$$

The above scheme has assumed that M_4 is positive. Conditions for this need to be established. It turns out that $M_4 = 2h + E_0 k_1^2 k_2^2$ and from (3.3), it follows that

$$h^{-1} M_4 \Delta^* = 2(1-\cos\varphi) \left\{ 1 - \frac{\sin 2\theta}{2\theta} \right\} - (\theta \leftrightarrow \varphi). \tag{B.2}$$

With $\varphi > \theta$, $\Delta^* > 0$, we thus only need the conditions under which

$$F(\theta) = \frac{1 - \sin 2\theta/2\theta}{1 - \cos\theta}$$

is a decreasing function of θ. A graphical examination reveals the requirement $\varphi < \pi$. Moreover, from (B.2) we may now write

$$h^{-1} M_4 = \frac{F(\theta) - F(\varphi)}{\cos\theta - \cos\varphi} \tag{B.3}$$

and the largest value of λ for which $F(\theta) - \lambda\cos\theta$ remains a decreasing function on $[0,\pi]$ appears to be λ=0.25. Thus $M_4 > h/4$. Suppose next that $\xi_0 < h$. Manipulating (B.1) results in the alternative inequality $M_4 < \rho h/4$ where

$$\rho^{-1} = \tfrac{5}{4} \left(1 - \frac{\varphi^2 + \theta^2}{30} \right).$$

The condition which ensures a contradiction is therefore, $\varphi^2 < 3$.

We next turn our attention to the interval $[0,h]$ (or, equivalently $[-h,0]$). This case is much more difficult to consider with inequalities written from terminated Taylor expansions, but another method has not been found. Moreover, without going to extraordinary lengths, the restriction on φ will have to be strengthened to $\varphi < 0.43$, for this interval. Severe numerical testing has indicated that a result on $\varphi < \sqrt{\pi}$ should be possible; however the essential part of any result is that the upper bound on φ is *independent* of the step length h, thus ensuring that a *definite* Peano kernel is always possible regardless of the size of k_1, k_2.

We write $\phi_2(x)$ as a Taylor expansion about $x=0$

$$\phi_2 = (k_1 A_1 + k_2 C_1 - (k_1 k_2)^{-2})x - \tfrac{1}{6}(k_1^3 A_1 + k_2^3 C_1)x^3 + E_T \tag{B.4}$$

where the "tail" E_T is to be proved positive in $[0,h]$. With that established, the positivity (negativity) of K on $[-2h,0]$ ($[0,2h]$) then follows by proving that the positive zero of the leading cubic above occurs for $x > h$. Throughout we shall require a number of trigonometric inequalities of the type

$$\tfrac{1}{2}(\varphi^2-\theta^2)\left(1-\frac{\varphi^2+\theta^2}{12}\right) < \cos\theta - \cos\varphi < \tfrac{1}{2}(\varphi^2-\theta^2)$$

which are trivial to establish when, as in our case, $0 < \theta < \varphi \leqslant 1$. In the interest of space, not all inequalities used are written explicitly. However, note from (3.4) and further expansions, that we have

$$1+\tfrac{1}{6}(\varphi^2+\theta^2)-\tfrac{1}{80}(\varphi^2+\theta^2)^2 < \frac{1}{4\Delta^*}(\varphi^2-\theta^2)\varphi^2\theta^2.$$

Now observe, by considering similar inequalities for e.g. $2\cos 2\theta - \sin 2\theta/\theta$ in (3.3), that $E_1 < 0$. From consideration of the last two conditions in Appendix A it then follows that $D_1 < 0$. The series for E_T may be written

$$E_T = -D_1\sum_{n=2}^{\infty}\frac{(-)^n}{(2n)!}\{k_2^{2n-2}-k_1^{2n-2}\}x^{2n}+\sum_{n=2}^{\infty}\frac{(-)^n}{(2n+1)!}\{A_1k_2^{2n+1}+C_1k_1^{2n+1}\}x^{2n+1}$$

and the first series remains positive if $0 < x < h$, by taking pairs of terms as before. The second series proves more challenging since A_1 and C_1 will be seen to differ in sign. We can proceed however, by induction. The inductive hypothesis is that

$$A_1\theta^{2m+1}+C_1\varphi^{2m+1} > \frac{A_1\theta^{2m+3}+C_1\varphi^{2m+3}}{(2m+2)(2m+3)},\quad \forall m \leqslant n-1, \tag{B.5}$$

and we consider truth for $m = 0$ below, in conjunction with estimating the zero of the cubic.

We have the identity

$$\begin{aligned} A_1\theta^{2m+3}+C_1\varphi^{2m+3} &\equiv (A_1\theta^{2m+1}+C_1\varphi^{2m+1})(\varphi^2+\theta^2)-\varphi^2\theta^2(A_1\theta^{2m-1}+C_1\varphi^{2m-1})\\ &< (A_1\theta^{2m+1}+C_1\varphi^{2m+1})\left\{\varphi^2+\theta^2-\frac{\varphi^2\theta^2}{2m(2m+1)}\right\}\end{aligned}$$

by the hypothesis. Thus, (B.5) holds for $m = n$, provided

$$\frac{\varphi^2\theta^2}{2n(2n+1)} < (\varphi^2+\theta^2) < \frac{\varphi^2\theta^2}{2n(2n+1)}+(2n+2)(2n+3),$$

which is clearly satisfied under our assumptions restricting θ, φ.

We can then turn our attention to the main inequality arising from (B.4) required to show that K is *definite* on $[-2h,0]$ and $[0,2h]$, namely

$$6(A_1\theta+C_1\varphi) > \frac{6h^5}{\varphi^2\theta^2}+A_1\theta^3+C_1\varphi^3. \tag{B.6}$$

After some elaborate algebra using the equations written in Appendix A, we have that

$$(\varphi^2-\theta^2)\{A_1\theta(6-\theta^2)+C_1\varphi(6-\varphi^2)\} = \theta^2\varphi^2(E_1-E_0)S_1+(E_0\theta^2\varphi^2+2h^5)S_2+Ch^5, \tag{B.7}$$

where

$$S_N \equiv 6\sin N\theta/\theta - \theta\sin N\theta - \theta \leftrightarrow \phi \quad \text{and} \quad C \equiv (6/\theta^2 - 1)\cos 2\theta - \theta \leftrightarrow \phi.$$

It is also worth noting the simplifications

$$\Delta^*(E_0\theta^2\varphi^2 + 2h^5) = 2h^5(1-\cos\varphi)\left(1 - \frac{\sin 2\theta}{2\theta}\right) - \theta \leftrightarrow \phi,$$

$$\Delta^*(E_1 - E_0)\theta^2\varphi^2 = 2h^5(1-\cos\varphi)\left(\frac{\sin 2\theta}{2\theta} - \cos 2\theta\right) - \theta \leftrightarrow \phi.$$

We can note further inequalities required:

$$\{S_1, S_2\} > (\varphi^2 - \theta^2)\left\{\{2, 10\} - \{\tfrac{13}{60}, \tfrac{44}{15}\}(\varphi^2 + \theta^2)\right\}, \; C > \frac{6(\varphi^2 - \theta^2)(1 - \varphi^2\theta^2)}{\varphi^2\theta^2},$$

$$\Delta^*(E_1 - E_0)\theta^2\varphi^2 > h^5\varphi^2\theta^2\left\{\tfrac{19}{45}(\varphi^2 - \theta^2) - \tfrac{137}{1890}(\varphi^4 - \theta^4)\right\}$$

and

$$\Delta^*(E_0\theta^2\varphi^2 + 2h^5) > h^5\varphi^2\theta^2\left\{\tfrac{7}{90}(\varphi^2 - \theta^2) - \tfrac{41}{3780}(\varphi^4 - \theta^4)\right\}.$$

Adding the various results written, we have finally, from (B.7) that

$$A_1\theta(6 - \theta^2) + C_1\varphi(6 - \varphi^2) > h^5\left\{4(\tfrac{73}{45} - \tfrac{1907}{6300}(\varphi^2 + \theta^2) - \tfrac{5161}{75\,600}(\varphi^2 + \theta^2)^2) + \frac{6(1 - \varphi^2\theta^2)}{\varphi^2\theta^2}\right\}.$$

The requirement which will validate (B.6) is therefore

$$770 > 1907(\varphi^2 + \theta^2) + \tfrac{5161}{12}(\varphi^2 + \theta^2)^2$$

and this is certainly satisfied if $0 < \theta \leqslant \varphi \leqslant 0.43$.

Finally observe that, with (B.6) established, the validity is also established of (B.5) for the case $m = 0$.

Appendix C

We seek to estimate (asymptotically as $h \to 0$) $\tilde{L}_3(b)$ as defined in Section 4. Thus, we have to compute two integrals, one on $[0, h]$ using ϕ_1 and one on $[h, 2h]$ using ϕ_0. Having already written an expansion for the latter on $[-2h, h]$ in Appendix B, we may exploit the *odd* parity of $K(x)$ and consider instead

$$I_1 \equiv -\int_{-2h}^{-h} \phi_0(x)\left\{\frac{x^4}{4!} + \frac{hx^3}{3!} - \frac{h^3x}{3}\right\} dx.$$

Since we require only a dominant term as $h \to 0$, it suffices to take the first two terms of ϕ_0 given. Thus,

$$\phi_0 \approx \frac{M_4}{4!}\xi^4 - \frac{1}{5!}\xi^5,$$

where $\xi = x + 2h$. We obtain the approximation $I_1 \approx -3803\,h^{10}/16\,329\,600$, having noted that $M_4 \approx \frac{14}{45}h$. The integral

$$I_2 \equiv \int_0^h \phi_1(x) \left\{ \frac{x^4}{4!} - \frac{hx^3}{3!} + \frac{h^3 x}{3} \right\} \mathrm{d}x,$$

on the other hand, is a little more tedious to estimate. Note however, that

$$A_1\theta + C_1\varphi - \frac{h^5}{\varphi^2\theta^2} = \left(\frac{E_1 - E_0}{6} + \frac{4E_0}{3} + \frac{2h^5}{\varphi^2\theta^2} \right) \varphi^2\theta^2 \approx -\tfrac{2}{135}h^5,$$

$$45(A_1\theta^3 + C_1\varphi^3) \approx -2h^5 \approx 2(A_1\theta^5 + C_1\varphi^5),$$

and that, beyond the fifth, no powers from the Maclaurin series for $\phi_1(x)$ will contribute to the leading order in h. We note that, correct to $\mathrm{O}(h^5)$,

$$\phi_1 = -\tfrac{2}{135}h^4 x + \tfrac{1}{135}h^2 x^3 - \tfrac{1}{90}hx^4 - \tfrac{1}{120}x^5$$

and we thus obtain the approximation $I_2 \approx -149h^{10}/201\,600$. Adding the two results, we have $\tilde{L}_3(b) \sim -124h^{10}/127\,575 \approx -0.00097h^{10}$.

We can similarly compute $\int_0^{2h} \tilde{L}_3(x)\,\mathrm{d}x$ using the kernel given in Section 4. The result is $\int_0^{2h} \tilde{L}_3(x)\,\mathrm{d}x \sim -5557h^{11}/5\,613\,300 \approx -0.00099h^{11}$.

References

[1] P. Bocher, H. De Meyer, V. Fack and G. Vanden Berghe, A parallel iterated correction mechanism for the numerical solution of Volterra equations, *APNUM*, to be published.

[2] P.J. Davis and P. Rabinowitz, *Methods of Numerical Integration* (Academic Press, New York, 2nd ed., 1984).

[3] H. De Meyer, J. Vanthournout and G. Vanden Berghe, On the error estimation for a mixed type of interpolation, *J. Comput. Appl. Math.* **32** (1990) 407–415.

[4] U.T. Ehrenmark, A three-point formula for numerical quadrature of oscillatory integrals with variable frequency, *J. Comput. Appl. Math.* **21** (1988) 87–99.

[5] U.T. Ehrenmark, On the automation of global error control for a two-parameter generalised Newton–Cotes rule, City of London Polytechnic, MDDS Working Paper No. 92/01 unpublished, 1992.

[6] U.T. Ehrenmark, On computing uniformly valid approximations for viscous waves on a plane beach, *J. Comput. Appl. Math.* **50** (1994) 263–281.

[7] S. Gan, Aspects of certain oscillatory functions, City of London Polytechnic, MDDS Project, unpublished, 1983.

[8] A. Ghizetti and A. Ossicini, *Quadrature Formulae* (Academic Press, New York, 1970).

[9] F.B. Hildebrand, *Introduction to Numerical Analysis.* (McGraw-Hill, New York, 1956).

[10] P. Köhler, On the error of parameter-dependent compound quadrature formulas, *J. Comput. Appl. Math.* **47** (1993) 47–60.

[11] A. Raptis and A.C. Allison, Exponential-fitting methods for the numerical solution of the Schrodinger equation, *J. Comput. Phys.* **6** (1970) 378–391.

[12] S. Rourke, Integrals with competing oscillatory components, City of London Polytechnic, MDDS Project, unpublished, 1987.

[13] M. Van Daele, H. De Meyer and G. Vanden Berghe, Modified Newton–Cotes Formulae for numerical quadrature of oscillatory integrals with two independent variable frequencies, *Internat. J. Comput. Math.* **42** (1992) 83–97.

[14] G. Vanden Berghe, H. De Meyer and J. Vanthournout, On a class of modified Newton–Cotes quadrature formulae based upon mixed-type interpolation, *J. Comput. Appl. Math.* **31** (1990) 331–349.

[15] G. Vanden Berghe and H. De Meyer, A finite-element estimate with trigonometric hat-functions for Sturm–Liouville eigenvalues, *J. Comput. Appl. Math.* **53** (1994) 389–396.